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CRYSTAL STRUCTURE OF SCANDENIN

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Scandenin ($C_{26}H_{26}O_6$), the major crystalline compound obtained from the roots of Derris Scandens, has been studied by many investigators[1-3] in view of its pronounced toxic properties. More recently, Rao and Khan[4] made a detailed chemical and spectroscopic study of the compound and concluded that it is a 2,3- disubstituted benzo-γ-pyranone derivative (Fig. 1). As regards the residue

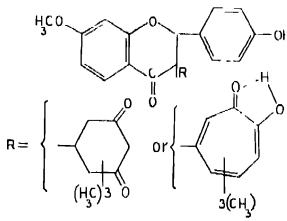

Fig. 1. Molecule of Scandenin

R in position 3, they proposed two alternative structures, namely, a tropolone ring or a dimedone ring. In order to find out which of these two structures is present, the authors have undertaken the structure analysis of scandenin. The present communication describes the results regarding its space group and unit cell dimensions.

The unit cell dimensions have been determined from rotation and zero layer Weissenberg photographs about the three crystallographic axes using CuK_α radiation Accurate values for the cell dimensions have been obtained by the least squares method using the data on the high angle reflections on Weissenberg photographs. The crystal is found to belong to the monoclinic system with the following cell dimensions.

$$a = 18.212\text{Å}, \quad b = 17.446\text{Å}, \quad c = 14.600\text{Å} \text{ and } \beta = 96°.$$

Examination of the zero layer and the higher layer equi-inclination Weissenberg photographs showed only two types of systematic absences, *hol* when *l* is odd and oko when *k* is odd which are consistent with the space group P_{2_1}/c.

The density of the crystal is determined by the floatation method using a mixture of nitrobenzene and *o*-dichlorobenzene The observed density 1.262 is found to be in good agreement with the value 1 246 calculated for 8 molecules per unit cell. The slightly higher value of the observed density may be due to the solvent of crystallisation We are now trying to introduce a heavy atom into the molecule and solve the structure by the heavy atom technique.

In conclusion, we wish to thank Professor N. V. Subba Rao for providing us with the scandenin crystals used in this investigation. One of us (P.V.R.) is grateful to the authorities of the Osmania University for the award of a research scholarship.

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